

Table 2. Structure factors for 'sum' and 'difference' reflections in static RbBr and CsI crystals

RbBr		<i>hkl</i>	111	311	331	200	220	222	400	440	444	800	10,0,0
LDA crystal			1.29	1.53	1.24	62.3	56.4	52.5	49.6	42.1	37.4	33.8	27.8
HF free ions			1.37	1.58	1.27	62.4	56.6	52.6	49.7	42.2	37.6	34.0	28.0
LDA free ions			1.39	1.56	1.26	62.3	56.5	52.5	49.6	42.1	37.4	33.8	27.8
CsI		<i>hkl</i>	100	111	210	110	200	220	400	431	530	541	444
LDA crystal			1.26	1.67	1.39	92.2	83.4	73.3	61.9	53.1	48.3	44.6	42.4
HF free ions			1.34	1.66	1.45	92.4	83.7	73.6	62.2	53.5	48.7	45.1	42.9
LDA free ions			1.35	1.63	1.41	92.2	83.5	73.3	61.9	53.1	48.3	44.6	42.4

The comparison of the LDA *crystal* structure factors and HF *free-ion* structure factors for the *static* crystals reveals very good agreement (within about 1%) for the 'sum' reflections, while for the 'difference' reflections the LDA factors are smaller than the HF factors – by about 6% for the lowest reflection. The LDA *free-ion* structure factors for the 'sum' reflections are practically identical to the LDA *crystal* structure factors, while for the 'difference' reflections the LDA *free-ion* factors are fairly close to the HF *free-ion* factors.

These results confirm the results reported by Böbel, Cortona, Sommers & Fumi (1983, 1985) for NaF and KCl crystals, and indicate a 'contraction' of the anion and a 'dilation' of the cation in passing from free ion to ion in crystal.

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Corrections and Additions

Acta Cryst. (1985). **A41**, 619

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Errors in the paper by Kramer & Neri [*Acta Cryst.* (1984), **A40**, 580–587] are corrected.

p. 585, § 7, first paragraph, last sentence should read: The enumeration of the dodecahedral faces is taken from Kramer (1982), except for an interchange of faces 1 and 6, and leads to Table 1.

p. 585, Table 4, column 'Class representative', third row should read: g_3, g_3^2 .

p. 585, Proposition 7.1, first equation should read:

$$D_{1'} = m^{-1} \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} m, \quad D_1 = D^{[311]'}, \quad D_2 = D^{[311]''}.$$

Reference

- KRAMER, P. (1982). *Acta Cryst.* **A38**, 257–264.